

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 270 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.43e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Simetryn</div> <div>Measured: 200</div> <div>Predicted: 244</div>	<div>Image not found</div> <div>Terbutylazine</div> <div>Measured: 209</div> <div>Predicted: 255</div>	<div>Image not found</div> <div>Propazine</div> <div>Measured: 251</div> <div>Predicted: 280</div>
<div>Image not found</div> <div>Atraton</div> <div>Measured: 437</div> <div>Predicted: 282</div>	<div>Image not found</div> <div>Ametryn</div> <div>Measured: 389</div> <div>Predicted: 390</div>	